Rosendo Valero

List of Publications by Year
in descending order

55 papers	3,657 citations	201658 27 h-index	161844 54 g-index
59 all docs	59 docs citations	59 times ranked	4833 citing authors

#	Article	IF	Citations
1	Artificial-intelligence-driven discovery of catalyst genes with application to CO2 activation on semiconductor oxides. Nature Communications, 2022, 13, 419.	12.8	45
2	Barnes Update Applied in the Gaussâ€“Newton Method: An Improved Algorithm to Locate Bond Breaking Points. Journal of Chemical Theory and Computation, 2021, 17, 996-1007.	5.3	6
3	Investigating the character of excited states in TiO₂nanoparticles from topological descriptors: implications for photocatalysis. Physical Chemistry Chemical Physics, 2020, 22, 3017-3029.	2.8	15
4	Quantum equilibration of the double-proton transfer in a model system porphine. Physical Chemistry Chemical Physics, 2020, 22, 22332-22341.	2.8	0
5	Morphology of TiO₂ Nanoparticles as a Fingerprint for the Transient Absorption Spectra: Implications for Photocatalysis. Journal of Physical Chemistry C, 2020, 124, 11819-11824.	3.1	8
6	Electronic Properties of Realistic Anatase TiO₂ Nanoparticles from G₀W₀ Calculations on a Gaussian and Plane Waves Scheme. Journal of Chemical Theory and Computation, 2019, 15, 5024-5030.	5.3	7
7	Interplay between the Gentlest Ascent Dynamics Method and Conjugate Directions to Locate Transition States. Journal of Chemical Theory and Computation, 2019, 15, 5426-5439.	5.3	3
8	Properties of Single Oxygen Vacancies on a Realistic (TiO₂)₈₄ Nanoparticle: A Challenge for Density Functionals. Journal of Physical Chemistry C, 2018, 122, 2413-2421.	3.1	22
9	Reliable and computationally affordable prediction of the energy gap of (TiO₂)_n(10 â‰¤nâ‰¤ 563) nanoparticles from density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 18907-18911.	2.8	18
10	Theoretical Modeling of Electronic Excitations of Gas-Phase and Solvated TiO₂ Nanoclusters and Nanoparticles of Interest in Photocatalysis. Journal of Chemical Theory and Computation, 2018, 14, 4391-4404.	5.3	24
11	An Empirical, yet Practical Way To Predict the Band Gap in Solids by Using Density Functional Band Structure Calculations. Journal of Physical Chemistry C, 2017, 121, 18862-18866.	3.1	165
12	Performance of theG₀W₀Method in Predicting the Electronic Gap of TiO₂Nanoparticles. Journal of Chemical Theory and Computation, 2017, 13, 3746-3753.	5.3	20
13	Adsorption and dissociation of molecular hydrogen on orthorhombic Î²-Mo2C and cubic Î´-MoC (001) surfaces. Surface Science, 2017, 656, 24-32.	1.9	50
14	Violation of DNA neighbor exclusion principle in RNA recognition. Chemical Science, 2016, 7, 3581-3588.	7.4	17
15	Intriguing Electrostatic Potential of CO: Negative Bond-ends and Positive Bond-cylindrical-surface. Scientific Reports, 2015, 5, 16307.	3.3	29
16	Spin Adapted versus Broken Symmetry Approaches in the Description of Magnetic Coupling in Heterodinuclear Complexes. Journal of Chemical Theory and Computation, 2015, 11, 1006-1019.	5.3	14
17	A molecular view of cisplatin's mode of action: interplay with DNA bases and acquired resistance. Physical Chemistry Chemical Physics, 2015, 17, 5155-5171.	2.8	39
18	An inelastic neutron scattering study of dietary phenolic acids. Physical Chemistry Chemical Physics, 2014, 16, 7491-7500.	2.8	10

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19	Applying vibrational spectroscopy to the study of nucleobases â€“ adenine as a case-study. New Journal of Chemistry, 2013, 37, 2691.	2.8	36
20	Polymorphism in Cisplatin Anticancer Drug. Journal of Physical Chemistry B, 2013, 117, 6421-6429.	2.6	34
21	Verdict: Time-Dependent Density Functional Theory â€œNot Guiltyâ€•of Large Errors for Cyanines. Journal of Chemical Theory and Computation, 2012, 8, 1255-1259.	5.3	122
22	Conformational behaviour of antioxidant chromones. A vibrational spectroscopy study. Vibrational Spectroscopy, 2012, 63, 325-337.	2.2	15
23	Quantitative integral cross sections for the H + CO2 â†' OH + CO reaction from a density functional theory-based potential energy surface. Physical Chemistry Chemical Physics, 2012, 14, 16699.	2.8	9
24	Photochemistry in a dense manifold of electronic states: Photodissociation of CH2ClBr. Journal of Chemical Physics, 2012, 137, 22A539.	3.0	17
25	Guanine: A Combined Study Using Vibrational Spectroscopy and Theoretical Methods. Spectroscopy, 2012, 27, 273-292.	0.8	50
26	Magnetic Coupling in Transition-Metal Binuclear Complexes by Spin-Flip Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2011, 7, 3523-3531.	5.3	52
27	How accurate are electronic structure methods for actinoid chemistry?. Theoretical Chemistry Accounts, 2011, 129, 657-666.	1.4	65
28	Density functional study of multiplicity-changing valence and Rydberg excitations of p-block elements: Delta self-consistent field, collinear spin-flip time-dependent density functional theory (DFT), and conventional time-dependent DFT. Journal of Chemical Physics, 2011, 135, 044118.	3.0	57
29	Density functional study of CO and NO adsorption on Ni-doped MgO(100). Journal of Chemical Physics, 2010, 132, 104701.	3.0	52
30	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 2071-2085.	5.3	383
31	Validation study of the ability of density functionals to predict the planar-to-three-dimensional structural transition in anionic gold clusters. Journal of Chemical Physics, 2009, 131, 064706.	3.0	70
32	Coupled-surface investigation of the photodissociation of NH3(Ã¹A″): Effect of exciting the symmetric and antisymmetric stretching modes. Journal of Chemical Physics, 2009, 130, 234303.	3.0	34
33	Consistent van der Waals Radii for the Whole Main Group. Journal of Physical Chemistry A, 2009, 113, 5806-5812.	2.5	1,325
34	Perspective on Diabatic Models of Chemical Reactivity as Illustrated by the Gas-Phase S_N2 Reaction of Acetate Ion with 1,2-Dichloroethane. Journal of Chemical Theory and Computation, 2009, 5, 2191-2191.	5.3	11
35	Valenceâ€“Bond Order (VBO): A New Approach to Modeling Reactive Potential Energy Surfaces for Complex Systems, Materials, and Nanoparticles. Journal of Chemical Theory and Computation, 2009, 5, 594-604.	5.3	11
36	Perspective on Diabatic Models of Chemical Reactivity as Illustrated by the Gas-Phase SN2 Reaction of Acetate Ion with 1,2-Dichloroethane. Journal of Chemical Theory and Computation, 2009, 5, 1-22.	5.3	45

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37	Adiabatic States Derived from a Spin-Coupled Diabatic Transformation: Semiclassical Trajectory Study of Photodissociation of HBr and the Construction of Potential Curves for LiBr⁺. Journal of Physical Chemistry A, 2008, 112, 5756-5769.	2.5	30
38	Good performance of the M06 family of hybrid meta generalized gradient approximation density functionals on a difficult case: CO adsorption on MgO(001). Journal of Chemical Physics, 2008, 129, 124710.	3.0	90
39	Performance of the M06 family of exchange-correlation functionals for predicting magnetic coupling in organic and inorganic molecules. Journal of Chemical Physics, 2008, 128, 114103.	3.0	208
40	A Diabatic Representation Including Both Valence Nonadiabatic Interactions and Spinâ^'Orbit Effects for Reaction Dynamics. Journal of Physical Chemistry A, 2007, 111, 8536-8551.	2.5	27
41	Improved direct diabatization and coupled potential energy surfaces for the photodissociation of ammonia. Theoretical Chemistry Accounts, 2007, 118, 9-24.	1.4	63
42	Identifying spectator bonds in modeling reactions: OH+COâ†'H+CO2. Chemical Physics Letters, 2006, 417, 43-47.	2.6	16
43	Rotational transitions and diffraction in D2 scattering from the LiF(001) surface: Theory and experiment. Journal of Chemical Physics, 2006, 124, 234707.	3.0	4
44	Nonadiabatic effects in Câ€"Br bond scission in the photodissociation of bromoacetyl chloride. Journal of Chemical Physics, 2006, 125, 194305.	3.0	20
45	Role of CO vibration in the complex-formingOH+COâ†'H+CO2reaction. Physical Review A, 2004, 70, .	2.5	21
46	New results for the OHâ€Š(Î½=0,j=0)+COâ€Š(Î½=0,j=0)â†'H+CO2 reaction: Five- and full-dimensional quantum dynamical study on several potential energy surfaces. Journal of Chemical Physics, 2004, 120, 4263-4272.	3.0	50
47	Classical trajectory study of the HOCO system using a new interpolated ab initio potential energy surface. Chemical Physics Letters, 2004, 393, 236-244.	2.6	40
48	Theoretical Reaction Dynamics Study of the Effect of Vibrational Excitation of CO on the OH + CO â†' H + CO2Reactionâ€. Journal of Physical Chemistry A, 2004, 108, 8672-8681.	2.5	27
49	Theoretical rate constants for the OH+COâ†'H+CO2 reaction using variational transition state theory on analytical potential energy surfaces. Journal of Chemical Physics, 2002, 117, 8736-8744.	3.0	27
50	Ab initio and kinetics study of the ground 1Aâ€³ potential energy surface of the O(1D)+N2Oâ†'2NO, N2+O2(a1Î"g) reactions. Chemical Physics Letters, 2002, 355, 123-132.	2.6	12
51	Ab initio and DFT study of the ground potential energy surface for the ()+â†'2 reaction. Chemical Physics Letters, 2001, 343, 119-129.	2.6	12
52	Ab initio1Aâ€² ground potential energy surface and transition state theory kinetics study of the O(1D)+N2Oâ†'2NO, N2+O2(aâ€‰1Î"g) reactions. Journal of Chemical Physics, 2001, 115, 7015-7031.	3.0	21
53	Ab initio ground potential energy surface (3Aâ€³) for the O(3P)+N2O reaction and kinetics study. Journal of Chemical Physics, 2001, 115, 2540-2549.	3.0	13
54	Ab initio and quasiclassical trajectory study of the N(2D)+NO(Xâ€Š2Î)â†'O(1D)+N2(Xâ€Š1Î£g+) reaction on the lowest 1Aâ€² potential energy surface. Journal of Chemical Physics, 2000, 113, 10983-10998.	3.0	28

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55	Theoretical investigation of the eight low-lying electronic states of thecis- andtrans-nitric oxide dimers and its isomerization using multiconfigurational second-order perturbation theory (CASPT2). Journal of Chemical Physics, 2000, 112, 6608-6624.	3.0	67